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Challenging models for flow in unsaturated, fractured rock through exploration of small scale processes

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Abstract. Fluid flow in unsaturated, fractured rock is studied with respect to applied environmental problems ranging from remediation of existing contaminated sites to evaluation of potential sites for isolation of hazardous or radioactive wastes. Spatial scales for such problems vary from meters to kilometers with temporal scales from months to tens of thousands of years. Because such scales often preclude direct physical exploration of system response and detailed site characterization, we are regularly forced to use our understanding (or misunderstanding) of the underlying physical processes to predict large scale behavior. It is essential that conceptual models used as the basis for prediction be firmly grounded in physical reality. In this paper, we provide examples of how recent advances in understanding of small-scale processes within discrete fractures may influence the behavior of fluid flow in fracture networks and ensembles of matrix blocks sufficiently to impact the formulation of intermediate-scale effective media properties. We also explore, by means of a thought experiment, how these same small-scale processes could couple to produce a large-scale system response inconsistent with current conceptual models of flow through unsaturated, fractured rock.

Introduction

The unique aspect of flow and transport through unsaturated, fractured rock is that two systems exhibiting vastly different hydraulic behavior (fractures and matrix) span the same domain. In both systems, fluid flow is primarily governed by capillary, gravity, and viscous forces, the effects of which are relatively well understood in unsaturated porous media (i.e., matrix). As a result, virtually all of our process-related uncertainty is associated with the incorporation of fractures into the system. This uncertainty is unfortunate, as the physical nature of fractures (relatively large, open, connected void spaces) implies that they will dominate system hydraulics whether they are flowing (conduits) or not (barriers).

A number of authors have contributed to the development of conceptual models for flow and transport through unsaturated fractured rock (e.g., Wang and Narasimhan, 1985; Evans and Nicholson, 1987; Pruess and Wang, 1987). However, the paucity of experimental data forced these, and subsequent authors to make many assumptions which have oversimplified the influence of fractures. In this paper, we consider results of laboratory experiments that elucidate small-scale processes within the plane of single fractures; we do not focus on the transfer of fluid between the fracture and the matrix, and refer the reader to Tidwell et al. (1995). Our intent is not to review, but to illustrate some of the implications of these recent results with respect to flow in fracture networks, ensembles of matrix blocks, and consequently the formulation of intermediate-scale effective media properties. To stimulate "cross-scale" discussion among researchers in this field, we also present a thought experiment in which small-scale processes interact to create large-scale system response that is very different than predicted by current unsaturated flow modeling.

Discrete Fracture Behavior and Potential Implications at Larger-Scales

Currently formulated continuum models for flow in unsaturated, fractured rock require definition of effective media properties. At the grid block scale, composite-continua models (e.g., Peters and Klavetter, 1988) require definition of a single effective media property that describes the combined behavior of both fractures and matrix. Dual-continua models (e.g., Barenblat and Zheltov, 1960) require definition of separate effective media properties for the fracture network and ensemble of matrix blocks within each grid block, as well as a transfer function between the two continua. In this section we first discuss current understanding of small-scale processes acting within discrete fractures and then consider the impact of these processes on the relative permeability of fracture networks and ensembles of matrix blocks.

Discrete fracture processes

For most natural gradient conditions in unsaturated, fractured rock, viscous forces will be small with respect to capillary and/or gravitational forces. Under such conditions, wetting-phase invasion of a horizontal fracture plane is controlled by capillary forces and phase accessibility. Complicated phase structures containing significant entrapped air form regardless of whether water enters the fracture from the matrix via contact points (Glass and Norton, 1992) or from the fracture edge (Nicholl and Glass, 1994); for both these situations, significant hysteresis in the pressure-saturation relations and phase structure have been measured. In experiments demonstrating air entrapment during in-plane wetting-phase invasion, fracture satiation was reached at saturations (S) of 0.6 to 0.7, with an associated decrease in fracture relative permeability (k_r) to less than 20% of the saturated value (Nicholl and Glass, 1994).

Percolation theory in two-dimensional networks (e.g., Wilkinson and Willemsem, 1983) suggests a percolation threshold pressure exists for each phase when fractures are much larger than the correlation length of the aperture field (where the field behaves as a random network). At pressures above this threshold, one phase spans the system and fully entraps the other to create a satiated condition. Therefore, in hor-

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izontal fractures, a bi-continua is precluded and relative permeability will display a discontinuous relationship with phase saturation; rising to the fully entrapped satiated value or abruptly dropping to zero near the percolation threshold pressure for each of the two phases. Percolation theory also predicts a fractal nature for the entrapped structure; the existence of phase structure at multiple scales implies a scale dependence for satiated fracture permeability (inverse with scale).

The dissolution or evolution of entrapped phase within the fracture alters phase structure. Gas depleted water dissolves air from the entrapped phase, increasing fluid saturation (and relative permeability) while supersaturated water evolves gases with opposite results. The gas exchange process proceeds at a rate dependent on the fluid flow rate, gas diffusion rate, and the gas concentration gradients within the water surrounding the entrapped bodies. These quantities in turn are defined by the phase structure and position within the flow field. Specific changes to the phase structure from gas dissolution are driven by accessibility concerns and hence will not necessarily drive the system towards a unique equilibrium structure (e.g., Glass and Nicholl, 1995).

At supply fluxes less than the gravity-driven saturated flux, gravity-driven "fingers" are expected to form in non-horizontal fractures; resulting wetted structures will be relatively compact and oriented along the gravitational gradient (Glass, 1990). Linear stability theory (Saffman and Taylor, 1958) has been used to analyze the breakup of a planar front advancing downward into porous media and smooth walled fractures (i.e., Hele-Shaw cells). However, fingers resulting from the cessation of ponded infiltration will be primarily defined by inflow boundary irregularities (finite amplitude perturbations) yielding finger widths different from those predicted by linear theory in either initially dry (Nicholl et al., 1994) or prewet fractures (Nicholl et al., 1993). In prewetted fractures, fingers are found to follow existing wetted structures formed by preceding fingers, thereby creating persistent pathways.

Instability of an advancing planar front is not required to form gravity-driven fingers. Individual fingers form from single point sources with relations for width and velocity dependent on supply rate, fracture conductivity, and fracture inclination (Nicholl et al., 1993). Point sources abound in individual fractures and fracture networks: wetted regions and contact points where water will enter the fracture from the matrix; low points along fracture intersections; irregularities in water inflow to a fracture or fracture network. Thus, for unsaturated flow in non-horizontal fractures, gravity-driven finger structures are expected, as long as fracture width (a function of supply rate, inclination, and fracture permeability) exceeds that of the finger.

We can assemble this understanding to postulate the behavior of relative permeability for single fractures that are significantly larger than both their aperture correlation lengths and the expected minimum finger width. At horizontal orientations, relative permeability will be a discontinuous function of saturation; zero at pressures below the percolation threshold and then jump to the satiated value. Fracture satiation, and hence permeability will be a function of wetting history and boundary conditions, as well as an inverse function of fracture size. If saturations above the percolation threshold are reached through gas dissolution, then , relative permeability will follow a power law relationship, $k_r \sim S^n$, with n = 4 or higher (Glass and Nicholl, 1995). In the vertical case, the influence of gravity is expected to produce an oriented phase structure that fully samples the aperture distribution; under such conditions, relative permeability will follow fracture saturation ($k_r \sim S$) with no fixed lower limit. The compact nature of fingers implies that fracture satiation, and thus satiated relative permeability, may be an increasing function of gravity; further exacerbating permeability differences between vertical and horizontal fractures. Also in contrast to horizontal fractures, gravity-induced anisotropy due to fingers suggests that simultaneous vertical flow of both phases will occur across a wide range of saturations, while horizontal flow will be restricted. As a further complication, relative permeability for all fracture inclinations will be a hysteretic function of pressure.

Implications: fracture network and matrix block ensemble permeability

At this time, experimental and numerical investigations of flow through unsaturated, fractured rock performed above the scale of an individual fracture, have not been designed to consider the discrete fracture behavior discussed above. Thamir et al. (1993) conducted an experiment in a fractured block that was not designed to allow such fracture behavior to be measured. Kwicklis and Healy (1993) have numerically studied the permeability of a 2-D network of fractures; however, the pressure/saturation and relative permeability relations used for the fractures did not incorporate satiated limits, hysteresis, or gravity-driven fingering in non-horizontal fractures.

If we assume that the fracture network is in some sense pervasive and fully averages the discrete behavior of individual fractures, we can use the directional behavior of fractures in the gravity field, as discussed above, to approximate at first order an anisotropic fracture network permeability. However, gravity-driven fingers tend to merge in individual fractures and thus, the possibility of large-scale finger confluence within the fracture network itself must also be considered. Fracture intersections could cause the confluence of fingered flow (much as we see in the laboratory when the bottom boundary of a fracture is left open to the air) with the formation of much stronger, more conductive fingers below. By analogy to studies in porous media (Glass et al., 1989), hysteretic response of fractures during fingering would limit the transfer of fluid from the finger both within the fracture plane, and through the matrix to other fractures.

Matrix flow for an ensemble of blocks will ultimately depend on hydraulic connection of individual matrix blocks across the fractures. For dry fractures, connection between adjacent matrix blocks is controlled by the inter-block contact points. Limited contact area severely restricts connectivity, and hence, reduces permeability of the ensemble. In partially-saturated fractures, fracture wetted structure (as discussed above) defines connection between matrix blocks, introducing a tortuosity term for matrix-matrix communication much different than that suggested by Wang and Narasimhan (1985). Blocks will have much less connection across vertical fractures due to fingering in the fracture plane than across horizontal fractures where the connection will most likely be fractal due to entrapment of air. Since fractures display strong hysteretic response to changes in matrix pressure, fractures at all angles are likely to form complicated sets of capillary barriers greatly constraining the transmission of flow from one fracture to other fractures via the matrix. The end result may allow formation of a preferential flow structure defined primarily by it's dynamic history rather than material properties.

Large-Scale System Behavior?

A major limitation of current effective continuum models for flow through unsaturated, fractured rock, is that focusing of flow and the associated formation of rapid transport pathways can only occur if significant (and perhaps unphysical) heterogeneity is inserted within the system model (e.g., Bovardsson et al., 1994). Above, we have discussed mechanisms that would permit formation of significant transport pathways within individual unsaturated fractures and fracture networks. These mechanisms initiate features smaller than the typical "grid block" scale (where effective properties are defined) that may network and form connected flow conduits at larger scales. The creation of these features within an unsaturated, fractured rock mass would be primarily process driven, and could occur in a system showing no heterogeneity at the grid block scale. In this section we use a simple thought experiment to demonstrate our point; noting that this is only one of many possible combinations of assumptions under consideration. We then provide observations from natural systems which offer evidence consistent with the outcome of this thought experiment.

Thought experiment

Consider a fractured rock unit of low matrix permeability/porosity that is dissected by a well connected fracture network with no specific preferential orientation. We assume that individual fractures exhibit an uninterrupted spatial extent that is both larger than the expected finger width and significantly larger than the aperture correlation lengths. As an initial condition, we assume that the fractures are dry and that the matrix is in a satiated state throughout the domain. The thought experiment begins by introducing steady flow at numerous discrete locations in the fracture network that are distributed along a horizontal plane passing through the system (e.g., non-uniform leakage from a perched zone or steady recharge focused into point sources by heterogeneity along a material boundary). The localized flow rates at the top input boundary are assumed to be high enough that the local potential gradient through the surrounding satiated matrix is unable to conduct the steady flow.

Gravity-driven fingers develop in inclined fractures near the input locations. Due to the hysteretic response of the fractures, once formed, these fingers persist. Fingered flow reduces interactions with the matrix blocks and fracture hysteretic response constrains the ability of the matrix to transmit fluid to other blocks and fractures. Thus, dissipation of the fingers via matrix interaction is severely limited. Heterogeneities in the fracture system (aperture, surface wettability, horizontal and sub-horizontal fractures) act to alter finger path, increasing the probability of finger contact and merger. On contacting a large aperture fracture that the finger cannot enter, the finger will be deflected by the capillary barrier and stop at its lowest point. Other fingers within the catchment zone of this barrier will merge above the barrier and feed into a confluence zone above this low point. The pressure within this local tension-satiated confluence zone builds until the water entry pressure of the barrier fracture is reached. Flow then crosses into the barrier fracture at one or more discrete points from which fingers form that continue downward to the next barrier/confluence zone. The process of merger due to the barrier/confluence mechanism allows the focusing of distributed flow sources into a small number of strong flow paths through the unsaturated, fractured rock mass.

It is important to note that the system-scale preferential flow paths described here are determined by the networking of small-scale processes (gravity-driven fingering, hysteretic fracture response, and barrier/confluence mechanisms). While we have observed the individual processes in the laboratory, experiments have not been conducted to verify their postulated networking. However, assuming this to be correct, the formation of large-scale preferential flow paths does not require any particular media or fracture network heterogeneity structure to be present. Therefore, spatial location of the primary flow paths may move in response to some system perturbations (i.e. excavation induced alteration of the stress field, climate change, tectonic activity) while remaining invariant under others (i.e. weather patterns). However, once a structure forms, over time it may alter system properties through geochemical processes to secure either its persistence or extinction in time. As currently formulated, continuum based models would dissipate flow from the point sources along the top boundary of our thought experiment, unless focusing is forced by significant material heterogeneity. Arbitrary definition of preferential flow structures through heterogeneous material properties creates features that may be unphysical and are not expected to respond to system perturbations in the same manner as those created by the coupling of small-scale flow processes as described in this thought experiment.

Reality of thought experiment

Insufficient data are available at this time to refute our postulated large-scale system behavior; in fact, the outcome of our thought experiment is consistent with observations at a number of natural fractured, unsaturated rock systems. The presence of localized fracture flow within otherwise unsaturated media is commonly encountered throughout the western United States. Specifically, flowing fractures located ~350 m below ground surface have been investigated at Rainier Mesa on the Nevada Test Site. Results suggest rapid fracture flow leading to travel times from the surface on the order of months to a few years (Russel et al., 1987). Similar studies are being performed on a series of flowing fractures located in a mining portal near the Apache Leap Site in Arizona (Bassett et al., 1994).

At Yucca Mountain, Nevada, saturation data suggest that many of the fractured welded units are at saturations above 0.6 at depth (A.L. Flint, personal communication). Since satiated values for welded tuff have been found to range from 0.4 to 0.9 (E.M. Kwicklis, personal communication) these units may be very near or at satiated saturations, thus greatly limiting matrix absorption of fracture flow as we assumed in our thought experiment. Geochemical data (Cl^{36}, tritium, C^{14}) collected at Yucca Mountain to date have provided evidence for possible rapid movement of some water within the unsaturated fractured rock. Liu et al., (1995) reports bomb pulse chlorine Cl^{36} at depths of over 350-450 m below surface. Locally elevated levels of tritium (420-430 m below surface) and C^{14} (369-435 m below surface) also indicate the presence of modern water at depth at Yucca Mountain (I.W. Yang, personal communication). While other causes for elevated concentrations of these elements are under evaluation, the fact that all three are found at depth is highly suggestive of rapid flow paths.

Currently accepted effective continuum models for flow in unsaturated, fractured rock do not support such rapid water movement without including extreme heterogeneity and boundary conditions. The combination of heterogeneity and boundary conditions could be considered to form a competing hypothesis to that proposed in our thought experiment above. It is most likely, however, that heterogeneity, boundary conditions and small-scale processes all combine to focus flow at the system scale. Since system response to perturbations (boundary conditions) will be dependent on the relative importance of heterogeneity and processes, it is important to resolve the significance of each. To test the relative importance of each to form preferential flow structures within unsaturated fractured rock will require carefully designed physical experiments and numerical simulations at a variety of scales and sites.

Conclusion

In order to formulate conceptual models for flow and transport through unsaturated, fractured rock, we must consider the processes affecting system response at a variety of scales. Small-scale (time, space) experimentation and analysis provides fundamental understanding of flow and transport processes. Coupling of these processes in a complex physical system yields hypothesized system responses that can be tested at the intermediate-scale where physical experiments and numerical simulations that explicitly include small-scale processes are designed. At large-scale, observations of both the natural system of interest and natural analog systems must be explored in the context of both small- and intermediate-scale understanding, with an ultimate goal of firmly grounding predictive models in physical reality.

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References

Barenblat, G.I., and I.P. Zheltov, On the basic flow equations of homogeneous liquids in fissured rocks (in Russian), *Dokl. Akad. Nauk SSSR*, 132,545-548, 1960.

Bassett, R.L., S.P. Neuman, T.C. Rasmussen, A. Guzman, G.R. Davidson, and C.F. Lohrstorfer, Validation studies for assessing unsaturated flow and transport through fractured rock, NUREG/CR-6203, U.S. Nuclear Regulatory Commission, 1994.

Bodvarsson, G., G. Chen, and C. Wittwer, Preliminary analysis of three-dimensional moisture flow within Yucca Mountain, Nevada, *Proc. 5th Ann. Int. Conf. on High Level Rad. Waste Mgmt.*, 2038-2047, Am. Nuc. Soc., Las Vegas, Nevada, May 22-26, 1994.

Evans, D.D., and T.J. Nicholson, Flow and transport through unsaturated rock: An overview, *Flow and Transport Through Unsaturated Fractured Rock,* D.D. Evans and T.J. Nicholson, editors, Geophysical Monograph 42, Am. Geophys. Union, Washington, DC, 1-10, 1987.

Glass, R.J., Laboratory research program to aid in developing and testing the validity of conceptual models for flow and transport through unsaturated porous media, *Proc. of the GEOVAL-90 Symposium on Validation of Geosphere Flow and Transport Models,* 275-283, Stockholm, Sweden, May 14-17, 1990.

Glass, R.J., and M.J. Nicholl, Quantitative visualization of entrapped phase dissolution within a horizontal flowing fracture, *Geophysical Research Letters*, this issue, 1995.

Glass, R.J. and D.L. Norton, Wetted region structure in horizontal unsaturated fractures: Water entry through the surrounding porous matrix, *Proc. 4th Ann. Int. Conf. on High Level Rad. Waste Mgmt.*, 717-726, Am. Nuc. Soc., Las Vegas, Nevada, April 12-16, 1992.

Glass, R.J., T.S. Steenhuis, and J-Y. Parlange, Mechanism for finger persistence in homogeneous unsaturated porous media: Theory and verification, *Soil Science*, 148, 60-70, 1989.

Kwicklis, E.M. and R.W. Healy, Numerical investigation of steady liquid water flow in a variably saturated fracture network, *Water Resources Res.*, 29(12), 4091-4102, 1993.

Liu, B., J. Fabryka-Martin, A. Wolfsberg, B. Robinson, and P. Sharma, Significance of apparent discrepancies in water ages derived from atmospheric radionuclides at Yucca Mountain, Nevada, *LANL report LA-UR-95-572*, 1995.

Nicholl, M.J., R.J. Glass, and H.A. Nguyen, Wetting front instability in an initially wet unsaturated fracture, *Proc. 4th Ann. Int. Conf. on High Level Rad. Waste Mgmt.*, 2061-2070, Am. Nuc. Soc., Las Vegas, Nevada, April 26-30, 1993.

Nicholl, M.J., R.J. Glass, and S.W. Wheatcraft, Gravity-Driven infiltration flow instability in non-horizontal unsaturated fractures, *Water Resources Res.*, 30(9), 2533-2546, 1994.

Nicholl, M.J. and R.J. Glass, Wetting phase permeability in a partially saturated horizontal fracture, *Proc. 5th Ann. Int. Conf. on High Level Rad. Waste Mgmt.,* 2007-2019, Am. Nuc. Soc., Las Vegas, Nevada, May 22-26, 1994.

Peters, R.R., and E.A. Klavetter, A continuum model for water movement in an unsaturated fractured rock mass, *Water Resources Res.*, 24(3), 416- 430, 1988.

Pruess, K., and J.S.Y. Wang, Numerical modeling of isothermal and nonisothermal flow in unsaturated fractured rock - A review, *Flow and Transport Through Unsaturated Fractured Rock,* D.D. Evans and T.J. Nicholson, editors, Geophysical Monograph 42, Am. Geophys. Union, Washington, DC, 11-22, 1987.

Russel, C.E., J.W. Hess, and S.W. Tyler, Hydrogeologic investigation of flow in fractured tuffs, Rainier Mesa, Nevada Test Site, in *Flow and Transport Through Unsaturated Fractured Rock,* Geophysical Monograph 42, American Geophysical Union, Washington D.C., 43-50, 1987.

Thamir, F., E.M. Kwicklis, and S. Anderson, Laboratory study of water infiltration into a block of welded tuff, *Proc. 4th Ann. Int. Conf. on High Level Rad. Waste Mgmt.*, 2071-2080, Am. Nuc. Soc., Las Vegas, Nevada, April 26-30, 1993.

Tidwell, V.C., R.J. Glass, and W.J Peplinski, Laboratory investigation of matrix imbibition from a flowing fracture, *Geophysical Research Letters*, this issue, 1995.

Wang, J.S.Y., and T.N. Narasimhan, Hydrologic mechanisms governing fluid flow in a partially saturated, fractured, porous medium, *Water Resources Res.*, 12(21), 1861-74, 1985.

Wilkensen, D. and J.F. Willemsen, Invasion percolation: A new form of percolation theory, *J. Phys. A:Math. Gen.*, 16, 3365-3376, 1983.

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